June 2015
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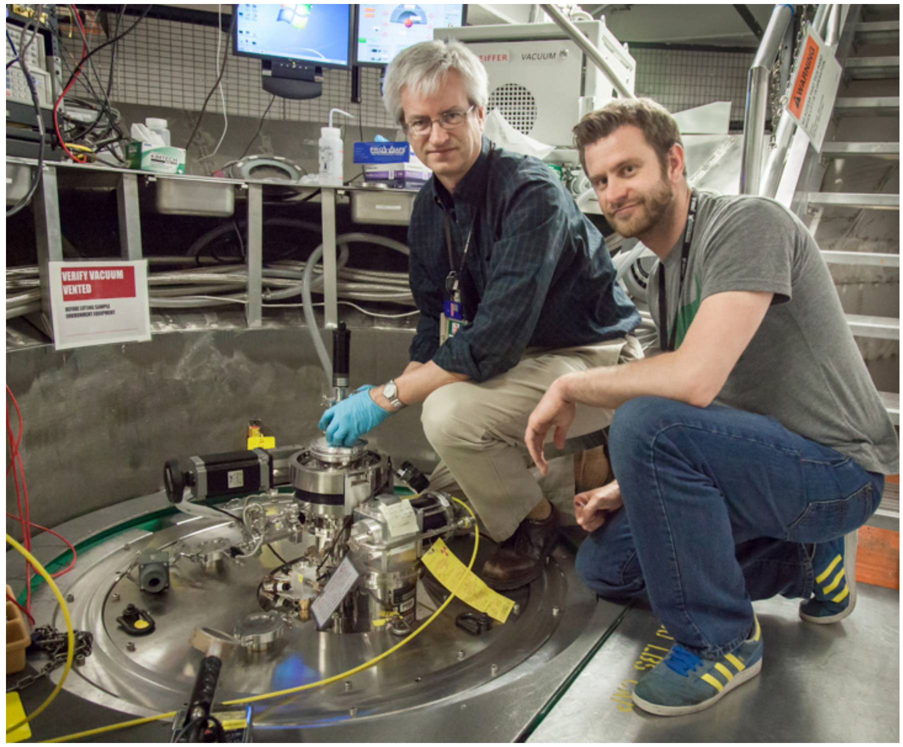
# MPA Materials Matter

INSIDE





**Marc Janoschek (far right) secures an average of 50 days a year of highly sought after neutron beam time at facilities around the globe. Here, he performs a break-through plutonium experiment at Oak Ridge National Laboratory with collaborator Doug Abernathy.**

Photo by Genevieve Martin, ORNL

> *"The processes that take the most frustration also give you the most reward afterward."*

## Marc Janoschek

### *Scattering neutrons to piece together the mystery of correlated electron materials*

*By Diana Del Mauro, ADEPS Communications*

In the spirit of the *Where's Waldo* series, imagine the adventures of Los Alamos materials physicist Marc Janoschek, whose globetrotting involves intense experiments for days at a time at neutron sources in the United States, Switzerland, France, and his native Germany. Janoschek most frequently works on uranium or cerium compounds, which exhibit mystifying physics similar to that of plutonium due to their complex electronic configuration. Look for him next in Japan and Australia.

"It's exciting to go to different places and work with different people and a different set of instruments," said Janoschek, a member of the Condensed Matter and Magnet Science group, who conducts his research at Los Alamos and elsewhere to get the best possible results.

MPA-CMMS "has an outstanding international reputation in strongly correlated electron physics. I knew all the papers, and I had met some of the scientists at conferences," said Janoschek, who was recruited in 2011 to head the group's neutron

*continued on page 3*

# From Rick's desk . . .

Thank you to everyone in MPA for your support and the warm reception after being selected as the MPA Deputy Division Leader. It is an honor to be in this position, working with Toni and the MPA leadership team to support the outstanding science and contributions from across the division. I continue to be impressed with the quality of research, science, and technologies that are part of MPA and look forward to an exciting future for our division.

As I write this we are in the midst of the Materials Capability Review. Recall this year's focus is on energetic materials and actinides and correlated electron materials. So far the response from the review committee has been highly complimentary, with praise for LANL's material science research. During each technical presentation, the committee was particularly interested in four main topics including: 1) relevance, 2) identification of the program sponsor, 3) identification of collaborators/competitors, and 4) specific details of the contribution. Sometimes our response to these four topics seems obvious; however, consistent reinforcement of relevance cannot be overstated.

"*In MPA, we continue to work aggressively to hire postdocs and outstanding early-career staff. Interestingly, our statistics for diversity have remained unchanged for the last several years. It is time to up our game.*"

The review also included working lunches with early- and mid-career employees. Attrition and retention across the Laboratory remain a concern. In MPA, we continue to work aggressively to hire postdocs and outstanding early-career staff. Interestingly, our statistics for diversity have remained unchanged for the last several years. It is time to up our game. We are now asking our staff to explore opportunities to broaden the candidate pool and include such information as part of the hiring package. Continued open discussions and awareness regarding diversity will hopefully help us understand the issue, create an environment for diversity, ensure that the process is objective, and hire the best candidate.

This year Antonya Sanders of MPA-CINT has agreed to be the MPA Student Liaison. She has an exciting summer planned with an introductory meeting, group activities, the student symposium, and concluding with a late summer picnic. ADEPS will also be conducting block training for new and returning students at the start of the summer. This training will probably be at TA-53: stay tuned for more details.

I look forward to learning more about the science in MPA, and as the new deputy it is going to be an exciting year. Summer is nearly upon us and I look forward to the influx of students with energy and enthusiasm to invigorate us all.

*MPA Deputy Division Leader Rick Martineau*

Rick

*Janoschek cont.*

scattering capability. "I loved the idea of a group that combines materials synthesis with a large suite of complementary characterization techniques to make progress in the understanding of novel materials. Another plus is I can just go across the street and have discussions with my theory colleagues."

Los Alamos Fellow Joe Thompson (MPA-CMMS) searched for three years for a neutron scattering expert who could use such expertise to expose the complexity of electronically correlated materials under various extreme conditions. He found Janoschek at the University of California, San Diego, where he was a postdoctoral fellow of Germany's Alexander von Humboldt Foundation. Thompson recruited him for a U.S. Department of Energy project on complex electronic materials relevant to research on emergent phenomena. "He was a great find," Thompson said. "He was worth the wait."

As part of Janoschek's doctoral thesis, he designed and built a first-of-its-kind polarimeter to enable magnetic structure and interaction studies in unprecedented detail. Two European neutron scattering centers use his novel device, for which he won the 2014 Wolfram-Prandl Prize. Janoschek said that experience taught him how to endure frustration—a resiliency he drew on recently to achieve what some in his field are calling "the most significant measurement on plutonium in a generation." It resolved the electronic ground state of delta plutonium for the first time, making significant progress on the understanding of plutonium's complex structural, electronic, and magnetic behavior. "The processes that take the most frustration also give you the most reward afterward," he said, summing up lessons he has learned. "Not so many things are impossible—it's just that our approach is from the wrong perspective."

It took two years—and the contributions of many—to develop uncrackable safety vessels and to complete the intricate experimental design, which he refined during trial runs at the Lujan Center using the Pharos inelastic neutron scattering instrument. "Neutron scattering experiments on plutonium compounds are exceptionally difficult because plutonium absorbs neutrons easily, which means the data are not very reliable," Janoschek said. "You have to use special tricks to circumvent that."

Today, Janoschek is excited about studying skyrmions, a continuation of his thesis research. He is pioneering ways to design materials with controllable functionality through these vortex-like magnetic objects, created and manipulated inside a material. Up to 100 nanometers in size, skyrmions offer the advantage of ultra-low power consumption. The research is funded by the Laboratory Directed Research and Development program and in line with the Lab's materials strategy and Department of Energy grand challenges in mesoscale science.

"Just as different combinations of atoms produce materials with different properties, different arrangements of skyrmions lead to distinct functionalities through coupling to electrical currents, magnetic and electrical fields, and temperature gradients," he said. "They have exceptional potential for computing, memory storage, and sensing applications."

## Marc Janoschek's favorite experiment

**What:** A neutron spectroscopy experiment on $CeRhIn_5$, which belongs to the 115 family of materials discovered here at Los Alamos National Laboratory.

**Why:** We wanted to determine the atomic-scale magnetic interactions between neighboring magnetic moments—that is, microscopic "compass needles" that sit on the cerium atoms. This information is required to understand the complex interplay of magnetic and electronic degrees of freedom believed to be at the heart of unconventional superconductivity, for which 115 materials serve as a test bench.

**When:** 2014

**Where:** Spallation Neutron Source, Oak Ridge National Laboratory

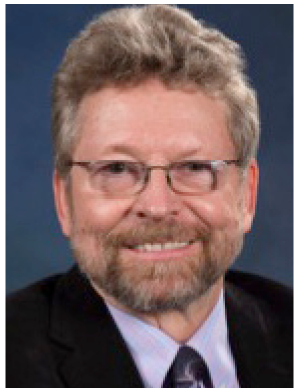
**Who**: Pinaki Das, Nirmal J. Ghimire, Kevin Huang, Filip Ronning, Eric Bauer, Joe Thompson (MPA-CMMS); Shizeng Lin and Christian Batista (Physics of Condensed Matter and Complex Systems, T-4); Georg Ehlers (Oak Ridge National Laboratory)

**How:** We used neutron spectroscopy, because it is the only method to obtain the strength of atomic-scale magnetic interactions reliably.

**The "a-ha moment:"** Surprisingly, the "a-ha moment" occurred before the experiment. This measurement was previously thought of as extremely difficult due to the strong neutron absorption of rhodium and indium. Still, Filip Ronning from my group kept on pestering me about this experiment for a year or so. When I was trying to prove to him that this experiment is impossible, I realized that we could design the sample in a special shape that made the experiment feasible! I love that I proved myself wrong.

## Laboratory Fellows recognize Rau and Zelenay for leadership, research

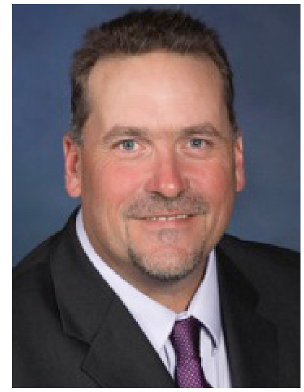
Jon Rau and Piotr Zelenay (both of Materials Synthesis and Integrated Devices, MPA-11) are recipients of 2015 Laboratory Fellows' prizes, which are awarded annually by the Laboratory Fellows to promote excellent technical achievements.



Zelenay received a Fellows' Prize for Research, which commends individuals for outstanding research performed at the Laboratory that was published within the last 10 years and has had a significant impact on its discipline or program. He is world-recognized in the area of inexpensive, nonprecious metal electrocatalysts intended to replace platinum in polymer electrolyte fuel cells for use in fuel cell electric vehicles. Zelenay led the use of nonprecious transition metal catalysts in a composite form, taking advantage of the latest developments in nanostructured materials engineering.

Zelenay earned doctoral and doctor of science ("habilitation") degrees in chemistry from the University of Warsaw, Poland, where he later served as a professor. He joined the Lab as a staff member in 1997.

Zelenay's previous honors include an award presented by the Energy Technology Division of The Electrochemical Society for his research on alternative energy sources, a DOE Hydrogen Program R&D Award in recognition of outstanding contributions to fuel cell technologies, the DOE "Energy 100" and "Energy @23" awards for fuel cells for transportation, the Fellowship of the Electrochemical Society, and a LANL Distinguished Performance Award. The Laboratory has given him the Patent and Licensing Award 10 times.



Rau received a Fellow's Prize for Leadership, which recognizes individuals for outstanding scientific and engineering leadership that serves the Laboratory mission. He has shown exemplary leadership in assembling and leading interdisciplinary teams of scientists to bring chemistry solutions and insight to bear on challenges in nuclear weapons. This approach was well received by numerous federal entities in the United States and in the United Kingdom. Rau also has mentored more than 25 young LANL staff members.

After completing a master's degree in chemistry from the University of Wisconsin-Madison, Rau joined the Laboratory in 1996. He leads materials-focused R&D projects to improve the safety of the enduring and future stockpile. He is also working to develop new processes to purify and recover plutonium-242 and other pure isotopes for the advancement of science and engineering.

Rau has also received two LANL Distinguished Performance Awards and three Defense Programs Awards of Excellence.

## Valence fluctuations trigger superconductivity in a plutonium compound

Los Alamos researchers have pinpointed the mechanism behind superconductivity in plutonium-cobalt-gallium-5 ($PuCoGa_5$), a compound with a surprisingly high superconducting transition temperature. The team leveraged the power of resonant ultrasound spectroscopy (RUS) to probe a sample from room temperature to 10 degrees (kelvin) above absolute zero. This discovery, in a heavy-fermion compound first identified at the Lab more than a decade ago, helps scientists understand which material properties lead to high superconducting transition temperatures. Their ultimate goal is to design a room-temperature superconductor. Room-temperature superconductors are of interest from a fundamental scientific perspective as well as for a variety of applications including superconducting magnets for cheaper and more powerful magnetic resonance imaging (MRI).

In ordinary members of the heavy-fermion superconductor family, scientists seek new superconductors by suppressing magnetism and activating superconductivity through spin fluctuations. However, $PuCoGa_5$ does not have the required magnetism to support this mechanism of superconductivity. According to Los Alamos research published in the *Proceedings of the National Academy of Sciences*, plutonium valence fluctuations are key to understanding the source of high-temperature superconductivity in $PuCoGa_5$, the highest $T_c$ superconductor of the heavy fermi-

**Probe used to locate the mechanism behind superconductivity in $PuCoGa_5$.**

*continued on next page*

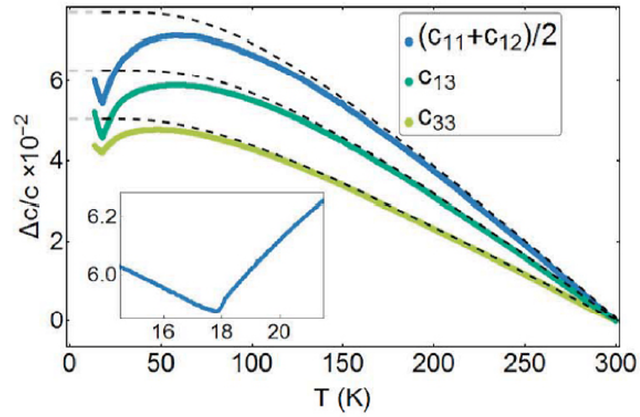
*Valence cont.*

ons, with a $T_c$ of 18.5 K. ($T_c$ refers to the critical temperature below which a superconductor must cool in order to exhibit this unusual state of matter in which electrical current flows without resistance as a result of the material's electrons acting in pairs.) A critical component of the discovery was the observation that the valence fluctuations disappear at $T_c$. This finding suggests that the same electrons that participate in the valence fluctuations also participate in superconductivity, providing a direct link between the two phenomena.

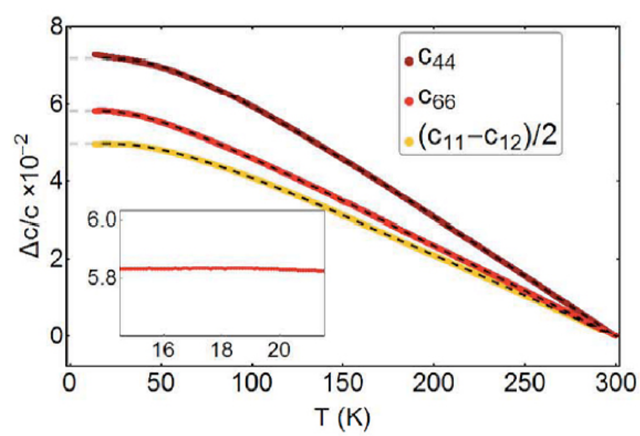
Elastic moduli measurements are a powerful tool for revealing valence fluctuations. Therefore, the Los Alamos researchers improved upon the sensitivity of RUS to resolve all the elastic moduli of $PuCoGa_5$ to low temperature in a way that was impossible with more traditional ultrasound techniques. Resonant ultrasound spectroscopy provides the highest absolute accuracy of any routine elastic modulus measurement technique, and it does this quickly on small samples. The National High Magnetic Field Laboratory at Los Alamos provides a RUS user facility for the general science community. The facility's capabilities range from 300 mK to 600 K and to 20 T. This provided a unique opportunity to explore the unusual valence of plutonium with a thermodynamic, symmetry-sensitive probe, allowing the scientists to find evidence for fluctuations of the plutonium 5f mixed-valence state.

The researchers found that the bulk modulus softens anomalously over a wide range in temperature above $T_c$. The elastic symmetry channel in which this softening occurs is characteristic of a valence instability. Therefore, the team identified the elastic softening with fluctuations of the plutonium 5f mixed-valence state. These valence fluctuations disappear when the superconducting gap opens at $T_c$. This result suggests that electrons near the Fermi surface play an essential role in the mixed-valence physics of this system and that $PuCoGa_5$ avoids a valence transition by entering the superconducting state. The lack of magnetism in $PuCoGa_5$ has made it difficult to reconcile with most other heavy-fermion superconductors, where superconductivity appears to be mediated by magnetic fluctuations. The new observations suggest that valence fluctuations play a critical role in the unusually high $T_c$ of $PuCoGa_5$.

Reference: "Avoided Valence Transition in a Plutonium Superconductor," *Proceedings of the National Academy of Sciences* **112**, 3285 (2015); published online before print March 3, 2015. Authors: Brad Ramshaw, Ross McDonald, Jon Betts, Chuck Mielke, and Eric Bauer (Condensed Matter and Magnet Science, MPA-CMMS); Arkady Shekhter (MPA-CMMS, now with NHMFL-Tallahassee); Jeremy Mitchell and Paul Tobash (Nuclear Materials Science, MST-16); and Albert Migliori (National Security Education Center, NSEC).




**The temperature-dependent elastic moduli of $PuCoGa_5$. The six elastic moduli in $PuCoGa_5$ can be grouped into two categories: shear moduli (below), which characterize how easily the material is distorted in a volume-preserving way (like stretching it along its diagonal); and compressional moduli (above), which characterize how easy it is to change the volume of the material. The shear moduli all show conventional behavior for a metal, becoming stiffer at low temperature. However, the compressional moduli stiffen to about 50 degrees above absolute zero, and then start to soften again. This unexpected behavior indicates valence fluctuations.**




Work at Los Alamos National Laboratory was performed under the auspices of the DOE, Basic Energy Sciences, Division of Materials Sciences and Engineering, and the LANL Laboratory Directed Research and Development program. This work was conducted at the National High Magnetic Field Laboratory, which the National Science Foundation and the State of Florida fund. The research supports the Lab's Energy Security mission area and Materials for the Future science pillar through the development of materials for energy applications.

*Technical contact: Brad Ramshaw*

*Soft matter in extremes*

# Using neutron scattering to determine the response of polymer films to high mechanical stresses

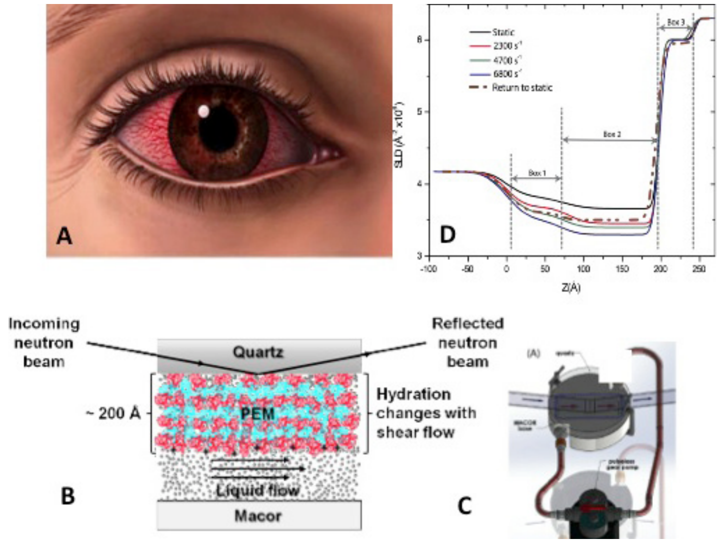
Although polymers are essential components in a range of items—from cosmetics and biocompatible surfaces of prosthetics to weapon components—fluidic shear's effect on the structure and properties of polymer thin films and mesoscopic assemblies has not been adequately investigated. Understanding these stresses is essential to increasing thin film applications, which range from materials science to biology and medicine, where bio-mechanical forces cause many critical processes.

Using the Surface Profile Analysis Reflectometer (SPEAR) beamline at the Los Alamos Neutron Science Center (LANSCE), Los Alamos researchers together with the University of South Florida and Alcon/Vision Care Company investigated fluidic shear's effect on polymer electrolytes thin films *via* neutron reflectometry (NR). NR is one of the few physical probes with sufficient nanometer-scale resolution, penetrability, and sensitivity that can address the properties of ultra-thin polymeric coatings in contact with flowing liquid and the stresses to which they are subjected.

Their research, appearing in *Langmuir,* raised important questions regarding the behavior of water molecules hydrating polymeric chains and their response to external stresses, especially in non-equilibrium states. Although water is one of the most common substances on Earth and is vital for many physico-chemical processes including all known life forms, its properties are still somewhat mysterious. Any result addressing its properties, especially in the nano- and meso-scales is, therefore, of great importance.

Neutron surface scattering, aligned with the capabilities of MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed facility for materials studies at the mesoscale, is an experimental approach that will address such time-dependent, soft-material problems.

For implantable biomaterials and tissue engineering, surface properties are highly important, influencing tissue and cellular events such as protein adsorption, cell adhesion, and inflammatory response. Creating composite nanostructures—by combining different poly-ions, nanoparticles, enzymes, proteins, and DNAs—increases the applications where such thin films can be used. The ability to estimate the damages/changes within such devices induced by shear stresses is, therefore, critical for their design and optimization. The fluidic shear stress can be significant: compared to ~500 $s^{-1}$ shear rates in a fire hose, fluid shear rates in the human body due to blood flow reach up to ~1500 $s^{-1}$ in capillaries and arterioles. Even more extreme, in the human ocular systems shear rates can reach up to 30000 $s^{-1}$ depending on tear film thickness (usually in μm range) and blink velocity (usually tens of cm/s).




**Neutron reflectometry's ability to probe fluidic shear's effects on polymer electrolyte thin films benefits a variety of fields where polymeric structures experience dramatic flow shear stresses. For example, (A) the surface of a contact lens can experience shear rates as strong as 30,000 $s^{-1}$ due to a moving eyelid and natural deficiencies in certain lubricating bio-molecules can lead to dry eye syndrome and inflamed conjunctiva. (B): Model system mimicking the cornea surface under the shear stress. (C): NR setup to measure effect of shear on the polymeric coating film. (D): NR results showing the polymeric meso-structure's response to the external fluid shear.**

Poly-electrolytes are charged water-soluble polymers conveniently used to coat solid surfaces in a technique where oppositely charged polymeric films are consecutively deposited through appropriate polymer-water solutions. The researchers investigated the response of these mesoscale thick films coating, consisting of alternating polyethylene imine and polystyrene sulfonate layers on quartz substrate, to fluid shear using neutron surface scattering probes. Given NR's high penetrability, which allows study of buried solid-liquid interfaces, favorable scattering contrast (polymers are mostly built of carbons and hydrogen with which neutrons strongly interact), angstrom-scale resolution, and lack of beam damage, neutrons are the ideal tool to study meso-scale structures in contact with fluids.

The NR results showed several unexpected results. For example, the researchers observed a monotonic decrease of the volume fraction of hydrating water inside the polymer film with increasing shear rate, and an approximate 7% uniform water volume fraction decrease throughout the film for the highest shear rate applied (~7000 $s^{-1}$). The water content decrease was not followed by any significant changes in the total polymer thickness, creating a significant negative osmotic pressure in the film. After the shear stress was

*continued on next page*

*Neutron cont.*

relieved, the polymers returned to their native state.

Reference: "Effects of Fluid Shear Stress on Polyelectrolyte Multilayers by Neutron Scattering Studies," by Saurabh Singh, Ann Junghans, Jaroslaw Majewski (Center for Integrated Nanotechnologies, MPA-CINT); Erik Watkins (Materials Synthesis and Integrated Devices, MPA-11); Yash Kapoor (Alcon, Vision Care R&D); and Ryan Toomey (University of South Florida), *Langmuir* **31** (9) 2015.

This work benefited from the use of the Lujan Center at LANSCE funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396. The research supports the Laboratory's national security mission area and Materials for the Future science pillar.

*Technical contact: J. Majewski*

## *Celebrating service*

Congratulations to the following MPA Division employees celebrating service anniversaries recently:

Tommy Rockward, MPA-11 ...................................... 15 years
Houtong Chen, MPA-CINT ....................................... 10 years
Carmen Espinoza, MPA-CMMS ............................... 10 years
Anirban Chaudhuri, MPA-11 ...................................... 5 years

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822 or kkippen@lanl.gov.
To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.

Los Alamos NATIONAL LABORATORY EST.1943



# HeadsUP!

## Your MPA WSST

**Who we are**
MPA WSST (Worker Safety and Security Team) is a grassroots collection of postdocs, technicians, and staff members with a goal of helping you get your work done by improving or resolving safety, security, and environmental problems.

**Informed source**
As a team we observe and develop solutions to current trends in safety and security issues within our division and directorate. Additionally, we aim to stay current of LANL safety requirements (policy) and help you do so as well, and watch for unanticipated changes within the policies that might inadvertently affect our operations.

*The MPA WSST is focused on helping our colleagues find solutions to safety and security issues within their work space, identify best practices within those work spaces, and help implement those practices across the division (through group-based solutions teams).*

**Resource for you**
The MPA WSST is focused on helping our colleagues find solutions to safety and security issues within their work space, identify best practices within those work spaces, and help implement those practices across the division (through group-based solutions teams). Additionally, we help MPA and EPS management councils to solve specific safety-related problems (e.g., injury analysis or reducing/simplifying live training requirements) with an eye toward real-world understanding of the laboratory setting. The goal of solutions teams is to help identify problems and resolve them on the spot. When the latter is not possible, the WSST will take these safety/security problems and bring them to the proper level of management for recognition and action, in addition to securing institutional funds when needed to effect those changes. Further, we are happy to act as a mediator between you and management during sensitive lab or incident inspections.

**MPA WSST points of contact for you**
- MPA-CMMS (Marcelo Jaime and Boris Maiorov)
- MPA-11 (Chris Romero and John Rowley)
- MPA-CINT (Jen Martinez)
- MPA-DO (Jeff Willis)

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